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**Americium Thermodynamic Data
for the EQ3/6 Database**

J. F. Kerrisk

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AMERICIUM THERMODYNAMIC DATA FOR THE EQ3/6 DATABASE

by

J. F. Kerrisk

ABSTRACT

Existing thermodynamic data for aqueous and solid species of americium have been reviewed and collected in a form that can be used with the EQ3/6 database. Data that are important in solubility calculations for americium at a proposed Yucca Mountain nuclear waste repository were emphasized. Conflicting data exist for americium complexes with carbonates. Essentially no data are available for americium solids or complexes at temperatures greater than 25°C.

I. INTRODUCTION

Americium is one of the radioactive waste elements that exists in spent fuel and reprocessed waste from nuclear reactors. Two isotopes of americium, ^{241}Am and ^{243}Am , are important radionuclides when considering geologic disposal of radioactive wastes.¹ For this reason, an understanding of the solubility and speciation of americium in aqueous solution will be necessary for geochemical modeling of a repository. At Los Alamos, the EQ3/6 chemical equilibrium computer programs are being used for geochemical modeling of Yucca Mountain, the proposed site being studied as part of the Nevada Nuclear Waste Storage Investigations.² No thermodynamic data for americium are currently available in the EQ3/6 database, but the literature has been reviewed and data are being collected and added to the database. This americium database will be used to:

- (1) assess the completeness and accuracy of existing thermodynamic data for americium,
- (2) estimate the solubility of americium in water at Yucca Mountain, and

- (3) guide future experimental work to answer important questions about americium behavior in aqueous solution.

II. TYPES OF THERMODYNAMIC DATA NEEDED

The data needed for chemical equilibrium calculations are equilibrium constants for reactions that involve the species of interest and the aqueous basis species. However, thermodynamic data are usually not compiled in this way. A program that is part of the EQ3/6 program package (MCRT) can be used to convert basic thermodynamic data, such as free energies of formation, entropies, and heat capacities, into the data needed for equilibrium calculations.³

A minimum requirement for aqueous species is the free energy of formation of the species from the elements in their standard states at one temperature. Data usually exist at 25°C, and an equilibrium constant can be calculated at that temperature by using the free energy of formation information. If, in addition, the entropy of the species or the entropy or enthalpy change of a reaction forming the species is known at the same temperature, a number of extrapolation techniques can be used to calculate equilibrium-constant data for the aqueous species over the 0 to 300°C temperature range.

For solids too, the minimum required data are the free energy of formation of the species from the elements in their standard states at one temperature. This information can be used to calculate an equilibrium constant at that temperature. If heat capacity data or the enthalpy change for a reaction forming the species are also available, equilibrium constants can be determined at other temperatures.

III. AMERICIUM DATA

In the literature, there are thermodynamic data for 26 aqueous species of americium. In addition, three other aqueous species that could be important have been postulated, but no thermodynamic data have been reported at this time. A listing of the species and accompanying data are contained in App. A, which is a copy of the input file MDAQS for the MCRT program. The file contains a list of references for the data and explains how specific data were chosen when conflicting sources were available. Emphasis was given to complexes of Am(III), which is the most likely oxidation state in dilute,

near-neutral solutions. Data were found for complexes of Am^{3+} with OH^- , CO_3^{2-} , F^- , Cl^- , SO_4^{2-} , PO_4^{3-} , and NO_3^- . At least one species in three other oxidation states (Am^{4+} , AmO_2^+ , and AmO_2^{2+}) was also included.

Thermodynamic data were found for only three solids of americium that would likely precipitate from aqueous solution: $\text{Am}(\text{OH})_3$, $\text{Am}(\text{OH})\text{CO}_3$, and $\text{Am}_2(\text{CO}_3)_3$. Solubility measurements have also been reported for solid AmO_2 , but the authors did not report equilibrium-constant data. A listing of the species and accompanying data are contained in App. B, which is a copy of the input file MDSOL for the MCRT program. The file contains a list of references for the data and explains how specific data were chosen when conflicting sources were available.

Appendix C contains a listing of the input file REAC for the MCRT program. REAC specifies the reactions involving the americium complexes and solids for which equilibrium constants will be determined by the MCRT program.

The output from the MCRT program is a file containing equilibrium-constant data for the reactions specified at 0, 25, 60, 100, 150, 200, 250, and 300°C. Appendix D contains a listing of this file, which also gives data for the species, the reaction being considered, and equilibrium constants as $\log_{10}K$. A value of 500 for $\log_{10}K$ indicates that no data are available at that temperature.

IV. DISCUSSION

The americium data collected in this review have been examined in an attempt to discover any discrepancies or inconsistencies. This is particularly important when data from more than one source are available or when the choice of other thermodynamic data influences the results of a particular experimenter.

Data for three of the hydrolysis products of Am^{3+} [$\text{Am}(\text{OH})^{2+}$, $\text{Am}(\text{OH})_2^+$, and $\text{Am}(\text{OH})_3$] have been reported by a number of experimenters (see App. A references). A fourth hydrolysis product [$\text{Am}(\text{OH})_4^-$] has been postulated by analogy with the rare earths, but no evidence for its existence has been published.⁴ Figure 1 shows a plot of $\log_{10}K$ for the reaction

Fig. 1. Americium hydrolysis products.

as a function of the number of ligands n .⁵⁻⁹ Three values have been shown for $n = 1$, four values for $n = 2$, and two values for $n = 3$. In addition, data for the analogous reaction for neodymium are shown.¹⁰ The Nd^{3+} ion is often used as a chemical analogue for Am^{3+} . The americium complexes appear to be more stable (larger $\log_{10}K$) than the comparable neodymium complexes. There was no clear reason to select the data of any one or two experimenters for these complexes; instead, average values were chosen and are shown by the dashed line in Fig. 1 (see comments in App. A for these species). In determining these average values, Shalinetz and Stepanov's data for $n = 1$ and $n = 2$ were disregarded as being out of line with the other reported data.⁵

There have been two recent reports of the solubility of solid $\text{Am}(\text{OH})_3$.^{8,11} Calculating a solubility product for $\text{Am}(\text{OH})_3$ requires knowledge of the hydrolysis equilibria; values for formation constants of hydrolysis products must either be assumed or determined as part of the work. Thus, the resulting solubility product is related to the choice of hydrolysis equilibrium constants; if either the solubility product or hydrolysis equilibrium constants are varied independently, incorrect predictions of solubility can result. Thermodynamic

data for solid $\text{Am}(\text{OH})_3$ were chosen as intermediate between the values reported by Silva¹¹ and Kim⁸ and were consistent with the choices of hydrolysis-product equilibrium constants described in the previous paragraph. Figure 2 shows the calculated solubility of solid $\text{Am}(\text{OH})_3$ compared with measured solubilities under the conditions of the two experimental measurements. Reported solubilities of americium from Edelstein¹² and Rai¹³ are also shown; the identity of the solid phase controlling solubility was not determined in either of these experiments.

The solubility of solid AmO_2 was also reported as a function of pH by Kim.⁸ Dissolution of AmO_2 involves the reduction of Am^{4+} to Am^{3+} and the formation of Am^{3+} complexes in solution. Thus, the solution Eh or some other measure of the redox state of the solution is necessary to interpret the solubility data in terms of equilibrium reactions. This work did not include redox measurements, so meaningful thermodynamic data cannot be derived from the solubility data.

Fig. 2. Americium solubility in 0.1 M NaClO_4 at 25°C.

Bidoglio⁶ and Lundqvist⁷ have experimentally determined complex formation between Am^{3+} , OH^- , and carbonate species. This work has recently been reviewed by Newton and Sullivan.¹⁴ The species identified in each work and their formation constants were used with the hydrolysis products of Am^{3+} (defined above) to calculate the predominant species in aqueous solution in the pH range from 6 to 11. Figure 3 shows the results for total carbonate of 2×10^{-3} M at ionic strength 0.1. These conditions are similar to the experimental conditions employed by the two investigators. It is apparent that the predominant species predicted from the two sets of formation constants are quite different. Bidoglio should have seen evidence for the AmCO_3^+ complex reported by Lundqvist, and Lundqvist should have observed the AmHCO_3^{2+} and $\text{Am}(\text{HCO}_3)_2^+$ complexes reported by Bidoglio. In the range of interest for water at Yucca Mountain (pH 6 to 8), the Bidoglio data predict that AmHCO_3^{2+} , $\text{Am}(\text{HCO}_3)_2^+$, and $\text{Am}(\text{CO}_3)_2^-$ are the primary aqueous species, whereas the Lundqvist data predict that Am^{3+} , AmCO_3^+ , $\text{Am}(\text{CO}_3)_2^-$, and two of the hydrolysis products (AmOH^{2+} and $\text{Am}(\text{OH})_2^+$) predominate. At this time, there are no other sources of information that would verify either of these two conflicting sets of data. The Lundqvist data have been employed for further calculations with EQ3/6 (see App. A), but this should be considered as an interim choice that will probably be modified as more data become available.

Evidence has been reported for two solids of americium with carbonate, $\text{Am}(\text{OH})\text{CO}_3$ and $\text{Am}_2(\text{CO}_3)_3$. Silva and Nitsche⁹ have recently reported a formation constant for solid $\text{Am}(\text{OH})\text{CO}_3$; they employed the complex formation constants of Lundqvist to analyze their data so their result was used directly. Their experiment was conducted at pH 6.1 and total carbonate of 2×10^{-4} M; neither of the carbonate complexes reported by Lundqvist is important under these conditions. If the carbonate complexes reported by Bidoglio had been used to analyze the data, significant aqueous concentrations of AmHCO_3^{2+} and $\text{Am}(\text{HCO}_3)_2^+$ would exist under these conditions and the reported formation constant would be different. Shiloh et al.¹⁵ reported evidence for the formation of solid $\text{Am}_2(\text{CO}_3)_3$ at high carbonate concentrations and high pH. The reported solubility of this material was used to estimate a solubility product for the solid. This estimate should be considered speculative at this time.

Fig. 3. Americium speciation in 0.1 M NaClO₄ at 25°C with 2×10^{-3} M total carbonate present.

Data for the formation of americium complexes with F^- , Cl^- , SO_4^{2-} , PO_4^{3-} , and NO_3^- are also listed in App. A. Where possible, thermodynamic data for these complexes were taken from the review by Phillips.¹⁶ Of these anions, only complexes with F^- appear to be of any importance in water at Yucca Mountain (see the following section). Formation constants for the fluoride complexes were taken from Phillips' review; they appear to be reliable data.

One aspect of essentially all the data collected for americium is that only 25°C data are available. For a thorough analysis of americium solubility, it may be necessary to extend data for important complexes and solids to higher temperatures.

V. SOLUBILITY OF AMERICIUM IN WATER FROM YUCCA MOUNTAIN

The solubility of americium will influence its rate of transport from a repository along water flowpaths toward the accessible environment. Calculations of americium solubility in water from Yucca Mountain were done using EQ3/6 and the thermodynamic data listed in App. D. Analyses of water from Well J-13 at the Nevada Test Site were used to define the water composition.¹⁷ The observed pH of Well J-13 water is approximately 7, and total carbonate is 2.3×10^{-3} M. The Eh was assumed to be 400 mV; this assumption should not affect the results because only the Am(III) oxidation state is expected in dilute, near-neutral solutions. It was assumed that the solid controlling solubility is $Am(OH)CO_3$. Figure 4 shows a plot of americium solubility and the predominant aqueous americium species from pH 6 to 8. At pH 6, a variety of species contribute to the aqueous americium content; at pH 7 to 8, $AmCO_3^+$ is the predominant aqueous species. With Well J-13 water in this pH range, the hydrolysis products are not important aqueous species. Solid $Am_2(CO_3)_3$ was also near saturation under these conditions. Although solid $Am(OH)_3$ was undersaturated, it could control solubility at higher pH or at lower total carbonate.

VI. RECOMMENDATIONS

This review has highlighted two problems with the available thermodynamic data that will be used to calculate americium solubility in aqueous solutions such as Well J-13 water. There is a conflict between the only two available sources of data for americium complexes with carbonate species. Because carbonate is the primary anion in water from Yucca Mountain, this conflict

Fig. 4. Americium solubility and speciation in Well J-13 water at 25°C.

must be resolved before americium solubility and speciation can be accurately determined for performance assessment. Further experimental work is needed to (a) identify the stoichiometry of the predominant aqueous complexes of americium with carbonate and (b) determine their formation constants. The second problem is that only data at 25°C are available for most americium species and compounds. Higher temperature data are needed, especially for solids controlling solubility and predominant aqueous species.

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APPENDIX A

Appendix A is a listing of the input file MDAQS for the MCRT program. This file contains thermodynamic data for aqueous species of americium.

MDAQSAM DATA FOR AQUEOUS COMPLEXES OF ALLPICIUM (SEE BOTTOM OF FILE)
 LAST REVISED 10/07/83

AM++++

ENTERED BY= J.F. KERRISK DATE= 09/01/83
 SOURCE= QUALITY=
 CHARGE= 4.0 TITR. FACTOR= 0.0 EQ/MOL
 ION TYPE= 1 ION SIZE= 0.0 A
 HYDR. NO.= 0.0
 1 CHEMICAL ELEMENTS=
 1.000 AM
 TEMP= 298.150 K PRESS= 1.000 BARS
 DELGO= -89.200 KCAL/MOL DELHO= -103.300 KCAL/MOL
 SO= -97.000 CAL/MOL/K SE= 3.560 CAL/MOL/K
 VO= 0.000 CC/MOL
 CP= 0.000 CAL/MOL/K
 NO T-P DATA GRID
 0 SPECIES IN REACTION=
 0.000 XX 0.000 XX 0.000 XX
 LOG K= 500.000 DELHOR= 500.000 KCAL/MOL
 DELSOR= 500.000 CAL/MOL/K

* SE TAKEN SAME AS PU+++.
 * FUGER AND GETTING (1976).

AM02+

ENTERED BY= J.F. KERRISK DATE= 09/01/83
 SOURCE= QUALITY=
 CHARGE= 1.0 TITR. FACTOR= 0.0 EQ/MOL
 ION TYPE= 1 ION SIZE= 0.0 A
 HYDR. NO.= 0.0
 2 CHEMICAL ELEMENTS=
 1.000 AM 2.000 D
 TEMP= 298.150 K PRESS= 1.000 BARS
 DELGO= -177.100 KCAL/MOL DELHO= -192.400 KCAL/MOL
 SO= -5.000 CAL/MOL/K SE= 2.180 CAL/MOL/K
 VO= 0.000 CC/MOL
 CP= 0.000 CAL/MOL/K
 NO T-P DATA GRID
 0 SPECIES IN REACTION=
 0.000 XX 0.000 XX 0.000 XX
 LOG K= 500.000 DELHOR= 500.000 KCAL/MOL
 DELSOR= 500.000 CAL/MOL/K

* SE FROM MCGLYNN AND SMITH (1961).
 * FUGER AND GETTING (1976).

AM02++

ENTERED BY= J.F. KERRISK DATE= 09/01/83
 SOURCE= QUALITY=
 CHARGE= 2.0 TITR. FACTOR= 0.0 EQ/MOL
 ION TYPE= 1 ION SIZE= 0.0 A
 HYDR. NO.= 0.0
 2 CHEMICAL ELEMENTS=
 1.000 AM 2.000 D
 TEMP= 298.150 K PRESS= 1.000 BARS
 DELGO= -140.400 KCAL/MOL DELHO= -155.800 KCAL/MOL
 SO= -21.000 CAL/MOL/K SE= 4.570 CAL/MOL/K
 VO= 0.000 CC/MOL
 CP= 0.000 CAL/MOL/K
 NO T-P DATA GRID
 0 SPECIES IN REACTION=
 0.000 XX 0.000 XX 0.000 XX
 LOG K= 500.000 DELHOR= 500.000 KCAL/MOL
 DELSOR= 500.000 CAL/MOL/K

* SE FROM MCGLYNN AND SMITH (1961).
 * FUGER AND GETTING (1976).

AM0H++

ENTERED BY= J.F. KERRISK DATE= 09/01/83
 SOURCE= QUALITY=
 CHARGE= 2.0 TITR. FACTOR= 0.0 EQ/MOL
 ION TYPE= 0 ION SIZE= 0.0 A
 HYDR. NO.= 0.0
 3 CHEMICAL ELEMENTS=
 1.000 AM 1.000 D
 TEMP= 298.150 K PRESS= 1.000 BARS

```

      DELGO=  -191.12  KCAL/MOL  DELHO=  500.000  KCAL/MOL
      SO=      500.000  CAL/MOL/K  SE=      0.000  CAL/MOL/K
      VO=      0.000  CC/MOL
      CP=      0.000  CAL/MOL/K
      NO T-P DATA GRID
      O SPECIES IN REACTION=
      0.000 XX          0.000 XX          0.000 XX
      LOG K=      500.000  DELHOR=  500.000  KCAL/MOL
      DELSOR=  500.000  CAL/MOL/K

*
* LUNDQVIST (1982), LOG K = -7.50 FOR AM+++ + H2O = AMOH++ + H+ AT I = 1.
* KIM (1983A), LOG K = 8.03 FOR AM+++ + OH- = AMOH++ AT I = 0.
* SHALINETS AND STEPANOV (1972), LOG K = 10.7 FOR AM+++ + OH- =
* AMOH++ AT I = 0.005; DATA SEEMS OUT OF LINE WITH OTHERS.
* USE AVERAGE OF KIM AND LUNDQVIST CORRECTED TO I = 0.
+-----+
AM(OH)2+
      ENTERED BY= J.F. KERRISK          DATE= 09/01/83
      SOURCE=          QUALITY=
      CHARGE=      1.0          TITR. FACTOR=  0.0 EQ/MOL
      ION TYPE=      1          ION SIZE=      0.0 A
      HYDR. NO.=      0.0
      3 CHEMICAL ELEMENTS=
      1.000 AM          2.000 O          2.000 H
      TEMP=      298.150 K          PRESS=      1.000 BARS
      DELGO=  -237.10  KCAL/MOL  DELHO=  500.000  KCAL/MOL
      SO=      500.000  CAL/MOL/K  SE=      0.000  CAL/MOL/K
      VO=      0.000  CC/MOL
      CP=      0.000  CAL/MOL/K
      NO T-P DATA GRID
      O SPECIES IN REACTION=
      0.000 XX          0.000 XX          0.000 XX
      LOG K=      500.000  DELHOR=  500.000  KCAL/MOL
      DELSOR=  500.000  CAL/MOL/K

*
* BIDOGLIO ET AL. (1983), LOG K = 12.845 FOR AM+++ + 2OH- = AM(OH)2+
* AT I = 0.2.
* SILVA (1982), LOG K = -16.7 FOR AM+++ + 2H2O = AM(OH)2+ + 2H+ AT
* I = 0.1.
* KIM (1983A), LOG K = 14.93 FOR AM+++ + 2OH- = AM(OH)2+ AT I = 0.
* SHALINETS AND STEPANOV (1972), LOG K = 20.9 FOR AM+++ + 2OH- =
* AM(OH)2+ AT I = 0.005; DATA SEEMS OUT OF LINE WITH OTHERS.
* USE AVERAGE OF BIDOGLIO, SILVA, AND KIM DATA CORRECTED TO I = 0.
+-----+
AM(OH)3
      ENTERED BY= J.F. KERRISK          DATE= 09/01/83
      SOURCE=          QUALITY=
      CHARGE=      0.0          TITR. FACTOR=  0.0 EQ/MOL
      ION TYPE=      0          ION SIZE=      0.0 A
      HYDR. NO.=      0.0
      3 CHEMICAL ELEMENTS=
      1.000 AM          3.000 O          3.000 H
      TEMP=      298.150 K          PRESS=      1.000 BARS
      DELGO=  -281.770  KCAL/MOL  DELHO=  500.000  KCAL/MOL
      SO=      500.000  CAL/MOL/K  SE=      0.000  CAL/MOL/K
      VO=      0.000  CC/MOL
      CP=      0.000  CAL/MOL/K
      NO T-P DATA GRID
      O SPECIES IN REACTION=
      0.000 XX          0.000 XX          0.000 XX
      LOG K=      500.000  DELHOR=  500.000  KCAL/MOL
      DELSOR=  500.000  CAL/MOL/K

*
* KIM (1983A), LOG K = 19.70 FOR AM+++ + 3OH- = AM(OH)3 AT I = 0.
* SILVA (1982), LOG K = -24.6 FOR AM+++ + 3H2O = AM(OH)3 + 3H+ AT
* I = 0.1.
* USE AVERAGE OF KIM AND SILVA DATA CORRECTED TO I = 0.
+-----+
AMCO3+
      ENTERED BY= J.F. KERRISK          DATE= 09/01/83
      SOURCE=          QUALITY=
      CHARGE=      1.0          TITR. FACTOR=  0.0 EQ/MOL
      ION TYPE=      1          ION SIZE=      0.0 A
      HYDR. NO.=      0.0
      3 CHEMICAL ELEMENTS=
      1.000 AM          3.000 O          1.000 C
      TEMP=      298.150 K          PRESS=      1.000 BARS
      DELGO=  -279.81  KCAL/MOL  DELHO=  500.000  KCAL/MOL
      SO=      500.000  CAL/MOL/K  SE=      0.000  CAL/MOL/K
      VO=      0.000  CC/MOL

```

```

      CP=          0.000 CAL/MOL/K
      NO T-P DATA GRID
      O SPECIES IN REACTION=
      0.000 XX          0.000 XX          0.000 XX
      LOG K=          500.000          DELHOR=          500.000 KCAL/MOL
      DELSOR=          500.000 CAL/MOL/K

*
* LUNDQVIST (1982), LOG K = 5.81 FOR AM+++ + CO3-- = AMCO3+ AT I = 1.0.
+-----+
AM(CO3)2-
  ENTERED BY= J.F. KERRISK          DATE= 09/01/83
  SOURCE=
  CHARGE=          -1.0          TITR. FACTOR=          0.0 EQ/MOL
  ION TYPE=          3          ION SIZE=          0.0 A
  HYDR. NO.=          0.0
  3 CHEMICAL ELEMENTS=
    1.000 AM          6.000 O          2.000 C
    TEMP=          298.150 K          PRESS=          1.000 BARS
    DELGO=          -412.14 KCAL/MOL          DELHO=          500.000 KCAL/MOL
    SO=          500.000 CAL/MOL/K          SE=          0.000 CAL/MOL/K
    VO=          0.000 CC/MOL
    CP=          0.000 CAL/MOL/K
  NO T-P DATA GRID
  O SPECIES IN REACTION=
  0.000 XX          0.000 XX          0.000 XX
  LOG K=          500.000          DELHOR=          500.000 KCAL/MOL
  DELSOR=          500.000 CAL/MOL/K

*
* BIDOGLIO ET AL. (1983), LOG K = 11.45 FOR AM+++ + 2CO3-- = AM(CO3)2-
* AT I = 0.2.
* LUNDQVIST (1983), LOG K = 9.72 FOR AM+++ + 2CO3-- = AM(CO3)2-
* AT I = 1.0.
* USE LUNDQVIST VALUE CORRECTED TO I = 0.
+-----+
AM(CO3)3---
  ENTERED BY= J.F. KERRISK          DATE= 09/01/83
  SOURCE=
  CHARGE=          -3.0          TITR. FACTOR=          0.0 EQ/MOL
  ION TYPE=          3          ION SIZE=          0.0 A
  HYDR. NO.=          0.0
  3 CHEMICAL ELEMENTS=
    1.000 AM          3.000 C          9.000 O
    TEMP=          298.150 K          PRESS=          1.000 BARS
    DELGO=          500.000 KCAL/MOL          DELHO=          500.000 KCAL/MOL
    SO=          500.000 CAL/MOL/K          SE=          0.000 CAL/MOL/K
    VO=          0.000 CC/MOL
    CP=          0.000 CAL/MOL/K
  NO T-P DATA GRID
  O SPECIES IN REACTION=
  0.000 XX          0.000 XX          0.000 XX
  LOG K=          500.000          DELHOR=          500.000 KCAL/MOL
  DELSOR=          500.000 CAL/MOL/K

*
* EVIDENCE FOR EXISTANCE FROM KIM (1983B), BUT NO PUBLISHED DATA.
* EVIDENCE OF RARE EARTH TRICARBONATE FROM FERRI ET AL. (1983), BUT
* NO DATA FOR AMERICIUM.
+-----+
AM(OH)CO3
  ENTERED BY= J.F. KERRISK          DATE= 09/01/80
  SOURCE=
  CHARGE=          0.0          TITR. FACTOR=          0.0 EQ/MOL
  ION TYPE=          0          ION SIZE=          0.0 A
  HYDR. NO.=          0.0
  4 CHEMICAL ELEMENTS=
    1.000 AM          4.000 O          1.000 H
    1.000 C
    TEMP=          298.150 K          PRESS=          1.000 BARS
    DELGO=          500.000 KCAL/MOL          DELHO=          500.000 KCAL/MOL
    SO=          500.000 CAL/MOL/K          SE=          0.000 CAL/MOL/K
    VO=          0.000 CC/MOL
    CP=          0.000 CAL/MOL/K
  NO T-P DATA GRID
  O SPECIES IN REACTION=
  0.000 XX          0.000 XX          0.000 XX
  LOG K=          500.000          DELHOR=          500.000 KCAL/MOL
  DELSOR=          500.000 CAL/MOL/K

*
* EVIDENCE FOR EXISTANCE FROM KIM (1983B), BUT NO PUBLISHED DATA.
+-----+
AM(OH)(CO3)2--

```



```

ENTERED BY= J.F. KERRISK          DATE= 09/01/83
SOURCE=                               QUALITY=
CHARGE= -2.0                        TITR. FACTOR= 0.0 EQ/MOL
ION TYPE= 3                          ION SIZE= 0.0 A
HYDR. NO.= 0.0
4 CHEMICAL ELEMENTS=
  1.000 AM          1.000 H          7.000 O
  2.000 C
  TEMP= 298.150 K      PRESS= 1.000 BARS
  DELGO= 500.000 KCAL/MOL DELHO= 500.000 KCAL/MOL
  SO= 500.000 CAL/MOL/K SE= 0.000 CAL/MOL/K
  VO= 0.000 CC/MOL
  CP= 0.000 CAL/MOL/K
NO T-P DATA GRID
0 SPECIES IN REACTION=
  0.000 XX          0.000 XX          0.000 XX
  LOG K= 500.000    DELHOR= 500.000 KCAL/MOL
  DELSOR= 500.000 CAL/MOL/K

*
* EVIDENCE FOR EXISTANCE FROM KIM (1983B), BUT NO PUBLISHED DATA.
* BIDDGLIO ET AL. (1983), LOG K = 15.57 FOR
* AM+++ + OH- + 2CO3-- = AM(OH)(CO3)2-- AT I = 0.2.
* DELGO = -457.00 KCAL/MOL; NOT USED IN DATAO AT THIS TIME.
+-----+
AM(OH)2CO3-
ENTERED BY= J.F. KERRISK          DATE= 09/01/83
SOURCE=                               QUALITY=
CHARGE= -1.0                        TITR. FACTOR= 0.0 EQ/MOL
ION TYPE= 3                          ION SIZE= 0.0 A
HYDR. NO.= 0.0
4 CHEMICAL ELEMENTS=
  1.000 AM          5.000 O          2.000 H
  1.000 C
  TEMP= 298.150 K      PRESS= 1.000 BARS
  DELGO= 500.000 KCAL/MOL DELHO= 500.000 KCAL/MOL
  SO= 500.000 CAL/MOL/K SE= 0.000 CAL/MOL/K
  VO= 0.000 CC/MOL
  CP= 0.000 CAL/MOL/K
NO T-P DATA GRID
0 SPECIES IN REACTION=
  0.000 XX          0.000 XX          0.000 XX
  LOG K= 500.000    DELHOR= 500.000 KCAL/MOL
  DELSOR= 500.000 CAL/MOL/K

*
* EVIDENCE FOR EXISTANCE FROM KIM (1983B), BUT NO PUBLISHED DATA.
+-----+
AMHCO3++
ENTERED BY= J.F. KERRISK          DATE= 09/01/83
SOURCE=                               QUALITY=
CHARGE= 2.0                      TITR. FACTOR= 0.0 EQ/MOL
ION TYPE= 1                        ION SIZE= 0.0 A
HYDR. NO.= 0.0
4 CHEMICAL ELEMENTS=
  1.000 AM          1.000 H          1.000 C
  3.000 O
  TEMP= 298.150 K      PRESS= 1.000 BARS
  DELGO= 500.000 KCAL/MOL DELHO= 500.000 KCAL/MOL
  SO= 500.000 CAL/MOL/K SE= 0.000 CAL/MOL/K
  VO= 0.000 CC/MOL
  CP= 0.000 CAL/MOL/K
NO T-P DATA GRID
0 SPECIES IN REACTION=
  0.000 XX          0.000 XX          0.000 XX
  LOG K= 500.000    DELHOR= 500.000 KCAL/MOL
  DELSOR= 500.000 CAL/MOL/K

*
* BIDDGLIO ET AL. (1983), LOG K = 4.79 FOR AM+++ + HCO3- = AMHCO3++ AT
* I = 0.2.
* DELGO = -291.14 KCAL/MOL; NOT USED IN DATAO AT THIS TIME.
+-----+
AM(HCO3)2+
ENTERED BY= J.F. KERRISK          DATE= 09/01/83
SOURCE=                               QUALITY=
CHARGE= 1.0                      TITR. FACTOR= 0.0 EQ/MOL
ION TYPE= 1                        ION SIZE= 0.0 A
HYDR. NO.= 0.0
4 CHEMICAL ELEMENTS=
  1.000 AM          2.000 H          2.000 C
  6.000 O
  TEMP= 298.150 K      PRESS= 1.000 BARS

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```

      DELGO=      500.000 KCAL/MOL      DELHO=      500.000 KCAL/MOL
      SO=         500.000 CAL/MOL/K      SE=         0.000 CAL/MOL/K
      VO=         0.000 CC/MOL
      CP=         0.000 CAL/MOL/K
      NO T-P DATA GRID
      O SPECIES IN REACTION=
      0.000 XX      0.000 XX      0.000 XX
      LOG K=      500.000      DELHOR=      500.000 KCAL/MOL
      DELSOR=      500.000 CAL/MOL/K
*
* BIDOGLIO ET AL. (1983), LOG K = 8.15 FOR AM+++ + 2HCO3- = AM(HCO3)2+
* AT I = 0.2.
* DELGO = -436.75 KCAL/MOL; NOT USED IN DATAO AT THIS TIME.
+-----+
AMF++
      ENTERED BY= J.F. KERRISK      DATE= 09/01/83
      SOURCE=      QUALITY=
      CHARGE=      2.0      TITR. FACTOR=      0.0 EQ/MOL
      ION TYPE=      1      ION SIZE=      0.0 A
      HYDR. NO.=      0.0
      2 CHEMICAL ELEMENTS=
      1.000 AM      1.000 F
      TEMP=      298.150 K      PRESS=      1.000 BARS
      DELGO=      -216.390 KCAL/MOL      DELHO=      500.000 KCAL/MOL
      SO=      -25.9 CAL/MOL/K      SE=      0.000 CAL/MOL/K
      VO=      0.000 CC/MOL
      CP=      0.000 CAL/MOL/K
      NO T-P DATA GRID
      O SPECIES IN REACTION=
      0.000 XX      0.000 XX      0.000 XX
      LOG K=      500.000      DELHOR=      500.000 KCAL/MOL
      DELSOR=      500.000 CAL/MOL/K
*
* AZIZ AND LYLE (1969).
* PHILLIPS (1982) LOG K = 4.3 FOR AM+++ + F- = AMF++ AT I = 0.
* SO FROM CHOPPIN AND UNREIN (1976), ERROR IN PAPER.
+-----+
AMF2+
      ENTERED BY= J.F. KERRISK      DATE= 09/01/83
      SOURCE=      QUALITY=
      CHARGE=      1.0      TITR. FACTOR=      0.0 EQ/MOL
      ION TYPE=      1      ION SIZE=      0.0 A
      HYDR. NO.=      0.0
      2 CHEMICAL ELEMENTS=
      1.000 AM      2.000 F
      TEMP=      298.150 K      PRESS=      1.000 BARS
      DELGO=      -287.940 KCAL/MOL      DELHO=      500.000 KCAL/MOL
      SO=      500.000 CAL/MOL/K      SE=      0.000 CAL/MOL/K
      VO=      0.000 CC/MOL
      CP=      0.000 CAL/MOL/K
      NO T-P DATA GRID
      O SPECIES IN REACTION=
      0.000 XX      0.000 XX      0.000 XX
      LOG K=      500.000      DELHOR=      500.000 KCAL/MOL
      DELSOR=      500.000 CAL/MOL/K
*
* AZIZ AND LYLE (1969).
* PHILLIPS (1982), LOG K = 7.4 FOR AM+++ + 2F- = AMF2+ AT I = 0.
+-----+
AMF3
      ENTERED BY= J.F. KERRISK      DATE= 09/01/83
      SOURCE=      QUALITY=
      CHARGE=      0.0      TITR. FACTOR=      0.0 EQ/MOL
      ION TYPE=      0      ION SIZE=      0.0 A
      HYDR. NO.=      0.0
      2 CHEMICAL ELEMENTS=
      1.000 AM      3.000 F
      TEMP=      298.150 K      PRESS=      1.000 BARS
      DELGO=      -359.630 KCAL/MOL      DELHO=      500.000 KCAL/MOL
      SO=      500.000 CAL/MOL/K      SE=      0.000 CAL/MOL/K
      VO=      0.000 CC/MOL
      CP=      0.000 CAL/MOL/K
      NO T-P DATA GRID
      O SPECIES IN REACTION=
      0.000 XX      0.000 XX      0.000 XX
      LOG K=      500.000      DELHOR=      500.000 KCAL/MOL
      DELSOR=      500.000 CAL/MOL/K
*
* AZIZ AND LYLE (1969).
* PHILLIPS (1982), LOG K = 10.6 FOR AM+++ + 3F- = AMF3 AT I = 0.

```

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+-----+
AMCL++
  ENTERED BY= J.F. KERRISK          DATE= 09/01/83
    SOURCE=                               QUALITY=
    CHARGE= 2.0          TITR. FACTOR= 0.0 EQ/MOL
    ION TYPE= 1          ION SIZE= 0.0 A
    HYDR. NO.= 0.0
    2 CHEMICAL ELEMENTS=
      1.000 AM          1.000 CL
        TEMP= 298.150 K          PRESS= 1.000 BARS
        DELGO= -176.080 KCAL/MOL          DELHO= 500.000 KCAL/MOL
        SO= 500.000 CAL/MOL/K          SE= 0.000 CAL/MOL/K
        VO= 0.000 CC/MOL
        CP= 0.000 CAL/MOL/K
    NO T-P DATA GRID
    0 SPECIES IN REACTION=
      0.000 XX          0.000 XX          0.000 XX
      LOG K= 500.000          DELHOR= 500.000 KCAL/MOL
      DELSOR= 500.000 CAL/MOL/K

*
* WARD AND WELCH (1956).
* PHILLIPS (1982), LOG K = 1.1 FOR AM+++ + CL- = AMCL++ AT I = 0.
+-----+

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AMCL2+
  ENTERED BY= J.F. KERRISK          DATE= 09/01/83
    SOURCE=                               QUALITY=
    CHARGE= 1.0          TITR. FACTOR= 0.0 EQ/MOL
    ION TYPE= 1          ION SIZE= 0.0 A
    HYDR. NO.= 0.0
    2 CHEMICAL ELEMENTS=
      1.000 AM          2.000 CL
        TEMP= 298.150 K          PRESS= 1.000 BARS
        DELGO= -208.09 KCAL/MOL          DELHO= 500.000 KCAL/MOL
        SO= 500.000 CAL/MOL/K          SE= 0.000 CAL/MOL/K
        VO= 0.000 CC/MOL
        CP= 0.000 CAL/MOL/K
    NO T-P DATA GRID
    0 SPECIES IN REACTION=
      0.000 XX          0.000 XX          0.000 XX
      LOG K= 500.000          DELHOR= 500.000 KCAL/MOL
      DELSOR= 500.000 CAL/MOL/K

*
* KHOPKAR AND NARAYANANKUTTY (1971)
* LOG K = 0.03 FOR AM+++ + 2CL- = AMCL2+ AT I = 1.
+-----+

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```

AMSD4+
  ENTERED BY= J.F. KERRISK          DATE= 09/01/83
    SOURCE=                               QUALITY=
    CHARGE= 1.0          TITR. FACTOR= 0.0 EQ/MOL
    ION TYPE= 1          ION SIZE= 0.0 A
    HYDR. NO.= 0.0
    3 CHEMICAL ELEMENTS=
      1.000 AM          4.000 O          1.000 S
        TEMP= 298.150 K          PRESS= 1.000 BARS
        DELGO= -326.060 KCAL/MOL          DELHO= 500.000 KCAL/MOL
        SO= 500.000 CAL/MOL/K          SE= 0.000 CAL/MOL/K
        VO= 0.000 CC/MOL
        CP= 0.000 CAL/MOL/K
    NO T-P DATA GRID
    0 SPECIES IN REACTION=
      0.000 XX          0.000 XX          0.000 XX
      LOG K= 500.000          DELHOR= 500.000 KCAL/MOL
      DELSOR= 500.000 CAL/MOL/K

*
* AZIZ ET AL. (1968).
* PHILLIPS (1982), LOG K = 3.6 FOR AM+++ + SD4-- = AMSD4+ AT I = 0.
+-----+

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AM(SD4)2-
  ENTERED BY= J.F. KERRISK          DATE= 09/01/83
    SOURCE=                               QUALITY=
    CHARGE= -1.0          TITR. FACTOR= 0.0 EQ/MOL
    ION TYPE= 3          ION SIZE= 0.0 A
    HYDR. NO.= 0.0
    3 CHEMICAL ELEMENTS=
      1.000 AM          8.000 O          2.000 S
        TEMP= 298.150 K          PRESS= 1.000 BARS
        DELGO= -505.920 KCAL/MOL          DELHO= 500.000 KCAL/MOL
        SO= 500.000 CAL/MOL/K          SE= 0.000 CAL/MOL/K
        VO= 0.000 CC/MOL
        CP= 0.000 CAL/MOL/K

```

```

NO T-P DATA GRID
O SPECIES IN REACTION=
  0.000 XX          0.000 XX          0.000 XX
    LOG K=          500.000          DELHOR=          500.000 KCAL/MOL
    DELSOR=          500.000 CAL/MOL/K

*
* AZIZ ET AL. (1968).
* PHILLIPS (1982), LOG K = 5.0 FOR AM+++ + 2SO4-- = AM(SO4)2- AT I = 0.
+-----+
AMH2PO4++
  ENTERED BY= J.F. KERRISK          DATE= 09/01/83
    SOURCE=          QUALITY=
    CHARGE=          2.0          TITR. FACTOR=          0.0 EQ/MOL
    ION TYPE=          1          ION SIZE=          0.0 A
    HYDR. NO.=          0.0
    4 CHEMICAL ELEMENTS=
      1.000 AM          4.000 O          1.000 P
      2.000 H
      TEMP=          298.150 K          PRESS=          1.000 BARS
      DELGO=          -417.090 KCAL/MOL          DELHO=          500.000 KCAL/MOL
      SO=          500.000 CAL/MOL/K          SE=          0.000 CAL/MOL/K
      VO=          0.000 CC/MOL
      CP=          0.000 CAL/MOL/K
    NO T-P DATA GRID
    O SPECIES IN REACTION=
      0.000 XX          0.000 XX          0.000 XX
        LOG K=          500.000          DELHOR=          500.000 KCAL/MOL
        DELSOR=          500.000 CAL/MOL/K

*
* LEBEDEV ET AL. (1979) LOG K = 2.73 FOR
* AM+++ + H2PO4- = AMH2PD4++ AT I = 0.
+-----+
AM(H2PO4)2+
  ENTERED BY= J.F. KERRISK          DATE= 09/01/83
    SOURCE=          QUALITY=
    CHARGE=          1.0          TITR. FACTOR=          0.0 EQ/MOL
    ION TYPE=          1          ION SIZE=          0.0 A
    HYDR. NO.=          0.0
    4 CHEMICAL ELEMENTS=
      1.000 AM          8.000 O          2.000 P
      4.000 H
      TEMP=          298.150 K          PRESS=          1.000 BARS
      DELGO=          -688.610 KCAL/MOL          DELHO=          500.000 KCAL/MOL
      SO=          500.000 CAL/MOL/K          SE=          0.000 CAL/MOL/K
      VO=          0.000 CC/MOL
      CP=          0.000 CAL/MOL/K
    NO T-P DATA GRID
    O SPECIES IN REACTION=
      0.000 XX          0.000 XX          0.000 XX
        LOG K=          500.000          DELHOR=          500.000 KCAL/MOL
        DELSOR=          500.000 CAL/MOL/K

*
* LEBEDEV ET AL. (1979) LOG K = 3.72 FOR
* AM+++ + 2H2PO4- = AM(H2PO4)2+ AT I = 0.
+-----+
AM(H2PO4)3
  ENTERED BY= J.F. KERRISK          DATE= 09/01/83
    SOURCE=          QUALITY=
    CHARGE=          0.0          TITR. FACTOR=          0.0 EQ/MOL
    ION TYPE=          0          ION SIZE=          0.0 A
    HYDR. NO.=          0.0
    4 CHEMICAL ELEMENTS=
      1.000 AM          12.000 O          3.000 P
      6.000 H
      TEMP=          298.150 K          PRESS=          1.000 BARS
      DELGO=          -960.11 KCAL/MOL          DELHO=          500.000 KCAL/MOL
      SO=          500.000 CAL/MOL/K          SE=          0.000 CAL/MOL/K
      VO=          0.000 CC/MOL
      CP=          0.000 CAL/MOL/K
    NO T-P DATA GRID
    O SPECIES IN REACTION=
      0.000 XX          0.000 XX          0.000 XX
        LOG K=          500.000          DELHOR=          500.000 KCAL/MOL
        DELSOR=          500.000 CAL/MOL/K

*
* MOSKVIN (1971) LOG K = 2.85 FOR
* AM+++ + 3H2PO4- = AM(H2PO4)3 AT I = 1.
+-----+
AM(H2PO4)4-
  ENTERED BY= J.F. KERRISK          DATE= 09/01/83

```

SOURCE= QUALITY=
 CHARGE= -1.0 TITR. FACTOR= 0.0 EQ/MOL
 ION TYPE= 4 ION SIZE= 0.0 A
 HYDR. NO.= 0.0
 4 CHEMICAL ELEMENTS=
 1.000 AM 16.000 D 4.000 P
 8.000 H
 TEMP= 298.150 K PRESS= 1.000 BARS
 DELGO= -1231.03 KCAL/MOL DELHO= 500.000 KCAL/MOL
 SO= 500.000 CAL/MOL/K SE= 0.000 CAL/MOL/K
 VO= 0.000 CC/MOL
 CP= 0.000 CAL/MOL/K
 NO T-P DATA GRID
 0 SPECIES IN REACTION=
 0.000 XX 0.000 XX 0.000 XX
 LOG K= 500.000 DELHOR= 500.000 KCAL/MOL
 DELSOR= 500.000 CAL/MOL/K

* MOSKVIN (1971) LOG K = 3.4 FOR AM+++
 * + 4H2PO4- = AM(H2PO4)4- AT I = 1.

AMNO3++
 ENTERED BY= J.F. KERRISK DATE= 09/01/83
 SOURCE= QUALITY=
 CHARGE= 2.0 TITR. FACTOR= 0.0 EQ/MOL
 ION TYPE= 1 ION SIZE= 0.0 A
 HYDR. NO.= 0.0
 3 CHEMICAL ELEMENTS=
 1.000 AM 3.000 D 1.000 N
 TEMP= 298.150 K PRESS= 1.000 BARS
 DELGO= -171.28 KCAL/MOL DELHO= 500.000 KCAL/MOL
 SO= 500.000 CAL/MOL/K SE= 0.000 CAL/MOL/K
 VO= 0.000 CC/MOL
 CP= 0.000 CAL/MOL/K
 NO T-P DATA GRID
 0 SPECIES IN REACTION=
 0.000 XX 0.000 XX 0.000 XX
 LOG K= 500.000 DELHOR= 500.000 KCAL/MOL
 DELSOR= 500.000 CAL/MOL/K

* KHOPKAR AND NARAYANANKUTTY (1971)
 * LOG K = 0.23 FOR AM+++ + NO3- = AMNO3++ AT I = 1.

AM(NO3)2+
 ENTERED BY= J.F. KERRISK DATE= 09/01/83
 SOURCE= QUALITY=
 CHARGE= 1.0 TITR. FACTOR= 0.0 EQ/MOL
 ION TYPE= 1 ION SIZE= 0.0 A
 HYDR. NO.= 0.0
 3 CHEMICAL ELEMENTS=
 1.000 AM 6.000 D 2.000 N
 TEMP= 298.150 K PRESS= 1.000 BARS
 DELGO= -198.48 KCAL/MOL DELHO= 500.000 KCAL/MOL
 SO= 500.000 CAL/MOL/K SE= 0.000 CAL/MOL/K
 VO= 0.000 CC/MOL
 CP= 0.000 CAL/MOL/K
 NO T-P DATA GRID
 0 SPECIES IN REACTION=
 0.000 XX 0.000 XX 0.000 XX
 LOG K= 500.000 DELHOR= 500.000 KCAL/MOL
 DELSOR= 500.000 CAL/MOL/K

* KHOPKAR AND NARAYANANKUTTY (1971)
 * LOG K = 0.13 FOR AM+++ + 2NO3- = AM(NO3)2+ AT I = 1.

AMO2HCO3
 ENTERED BY= J.F. KERRISK DATE= 09/01/83
 SOURCE= QUALITY=
 CHARGE= 0.0 TITR. FACTOR= 0.0 EQ/MOL
 ION TYPE= 0 ION SIZE= 0.0 A
 HYDR. NO.= 0.0
 4 CHEMICAL ELEMENTS=
 1.000 AM 1.000 H 1.000 C
 5.000 O
 TEMP= 298.150 K PRESS= 1.000 BARS
 DELGO= -320.520 KCAL/MOL DELHO= 500.000 KCAL/MOL
 SO= 500.000 CAL/MOL/K SE= 0.000 CAL/MOL/K
 VO= 0.000 CC/MOL
 CP= 0.000 CAL/MOL/K
 NO T-P DATA GRID

```

O SPECIES IN REACTION=
O.000 XX      O.000 XX      O.000 XX
LOG K=        500.000      DELHOR=    500.000 KCAL/MDL
DELSOR=      500.000 CAL/MDL/K
*
* MOSKVIN AND POZNYAKOV (1979) LOG K =
* AMO2+ + HCO3 = AMO2HCO3 AT I = 0.25.
+-----+
STOP.
MDAQSAM

```

DATA ON AQUEOUS COMPLEXES OF MANGANESE

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NOTATION--
-- DELGO = GIBBS ENERGY OF FORMATION
-- DELGOR = GIBBS ENERGY OF REACTION
-- DELHO = ENTHALPY OF FORMATION
-- DELHOR = ENTHALPY OF REACTION
-- SO = CONVENTIONAL ENTROPY
-- SE = INTERNAL ELECTRONIC ENTROPY
-- DELSOR = ENTROPY OF REACTION

```

NOTE THAT "500." IS ENTERED TO MEAN "NO DATA" FOR DELGO, DELHO, SO, LOG K, DELHO, AND DELSOR. NEVER ENTER ZERO OR LEAVE BLANK FOR THESE PARAMETERS UNLESS YOU MEAN TO USE AN ACTUAL VALUE OF ZERO.

IONIC STRENGTH CORRECTIONS NOTED IN THE ABOVE COMMENTS ON SPECIFIC SPECIES WERE MADE USING THE DAVIES EQUATION IN THE FORM

$$\text{LOG}(\text{GAMMA}) = 0.51 \times (Z^2) \left(\left(\frac{\text{SQRT}(I)}{(1 + \text{SQRT}(I))} \right) - (0.2 \times I) \right)$$

WHERE GAMMA IS THE ACTIVITY COEFFICIENT, Z IS THE CHARGE, AND I IS THE IONIC STRENGTH.

DATA FOR AQUEOUS SPECIES=

```

NAME= AN ALPHABETIC OR ALPHANUMERIC STRING
ENTERED BY= NAME OF PERSON WHO ENTERED DATA OR LAST REVISED IT
DATE= DATA OF ENTERING OR REVISING DATA
SOURCE= ALPHANUMERIC STRING IDENTIFYING A MAJOR SOURCE OF DATA. USE
"SEE BELOW" FOR MINOR SOURCES
QUALITY= ALPHANUMERIC STRING DESCRIBING THE PROBABLE ERROR IN GIBBS ENERGY
OR ITS EQUIVALENT, BASED ON SUBJECTIVE JUDGEMENT AND CHOSEN FROM
AMONG THE FOLLOWING (IN ORDER OF INCREASING VALUE)
    BAD - DEMONSTRABLY BAD DATA- DO NOT USE EXCEPT IN ILLUSTRATIVE
          CALCULATIONS
    POOR - LIKELY ERROR EXCEEDS A COUPLE OF KCAL OR SEVERAL KJ
    RESTRICTED - AD HOC FIT TO A PARTICULAR SITUATION; SEE NOTES
    SPECULATIVE - SPECIES NOT SHOWN CONCLUSIVELY TO EXIST
    UNCERTAIN - CHOSEN RATHER ARBITRARILY FROM DIVERGENT REPORTED
              VALUES
    UNSPECIFIED - NO QUALITY INFORMATION
    (BLANK) - EQUIVALENT TO UNSPECIFIED
    FAIR - LIKELY ERROR LESS THAN A COUPLE OF KCAL OR A FEW KJ
    GOOD - LIKELY ERROR LESS THAN ABOUT ONE KCAL OR FOUR KJ
THE CODE MUST BE MODIFIED TO ALLOW OTHER QUALITY PARAMETER INPUTS.
UNRECOGNIZED INPUTS ARE SET TO "ERROR". DATA FOR WHICH THE QUALITY
IS "RESTRICTED", "SPECULATIVE", OR "UNCERTAIN" MAY NUMERICALLY BE
"FAIR" TO "GOOD". THE MAJOR UNCERTAINTY ASSOCIATED WITH THESE VALUES
IS QUALITATIVE (I.E., UNCERTAINTY OF INTERPRETATION). DATA FOR WHICH
THE QUALITY IS "POOR" MAY BE QUITE SUFFICIENT FOR MAKING "GOOD"
CALCULATIONS- THIS DEPENDS ON THE SENSITIVITY OF THE RESULTS TO IT IN
ANY PARTICULAR APPLICATION.
CHARGE= ELECTRICAL CHARGE
TITRATION FACTOR= WEIGHTING FACTOR FOR PH 4.5 (METHYL ORANGE)
ALKALINITY
ION TYPE= CRISS-COBLE ION TYPE
0 NEUTRAL COMPLEX (MAY BE LEFT BLANK)
1 CATION (MAY BE LEFT BLANK)
2 SIMPLE ANION (MAY BE LEFT BLANK)
3 OXYANION
4 ACID OXYANION
ION SIZE= DEBYE-HUCKEL HYDRATED ION SIZE (FOR ACTIVITY COEFFICIENT
ESTIMATION)
HYDRATION NUMBER= NUMBER OF BOUND WATER MOLECULES NOT EXPLICITLY
SHOWN IN THE ASSUMED MOLECULAR FORMULA (FOR ACTIVITY COEFFICIENT

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ESTIMATION)
 TEMP= THE BASE POINT TEMPERATURE (K), USUALLY 298.15 K
 PRESS= THE BASE POINT PRESSURE (BARS), USUALLY 1 BAR
 DELGO= THE APPARENT STANDARD PARTIAL MOLAL GIBBS ENERGY AT THE
 BASE POINT
 DELHO= THE APPARENT STANDARD PARTIAL MOLAL ENTHALPY AT THE BASE POINT
 SO= THE CONVENTIONAL ENTROPY AT THE BASE POINT
 SE= THE INTERNAL ELECTRONIC ENTROPY; THIS FUNCTION IS ZERO EXCEPT FOR
 SOME ACTINIDE AND RARE EARTH SPECIES (IT IS USED IN CRISS-COBBLE
 METHOD TEMPERATURE EXTRAPOLATIONS)
 VO= THE PARTIAL MOLAL VOLUME AT THE BASE POINT; THERE IS NO CURRENT
 PROVISION FOR USING THIS INPUT IN THE CURRENT MCRT (AS OF 12/16/82)
 CP= THE PARTIAL MOLAL HEAT CAPACITY AT THE BASE POINT; THERE IS NO
 CURRENT PROVISION FOR USING THIS INPUT IN THE CURRENT MCRT (AS OF
 12/16/82)
 LOG K= LOG OF THE EQUILIBRIUM CONSTANT OF THE GIVEN REACTION AT THE
 BASE POINT
 DELHOR= ENTHALPY OF THE GIVEN REACTION AT THE BASE POINT
 DELSOR= ENTROPY OF THE GIVEN REACTION AT THE BASE POINT

REFERENCES

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STOP.

APPENDIX B

Appendix B contains a listing of the input file MDSOL for the MCRT program. This file contains thermodynamic data for solid species of americium.

MDSOLAM DATA FOR SOLIDS OF AMERICIUM (SEE BOTTOM OF FILE)
 LAST REVISED 10/07/83

AM(OH)3(C)

ENTERED BY= J.F. KERRISK DATE= 09/01/83
 SOURCE= QUALITY=
 3 CHEMICAL ELEMENTS=
 1.000 AM 3.000 O 3.000 H
 TEMP= 298.150 K PRESS= 1.000 BARS
 DELGO= -293.94 KCAL/MOL DELHO= 500.000 KCAL/MOL
 SO= 500.000 CAL/MOL/K VO= 0.000 CC/MOL
 1 HEAT CAPACITY RANGE(S) FOLLOW
 EQUATION= 0 CP OR A= 0.000 CAL/MOL/K
 B= 0.000 C= 0.000
 D= 0.000 E= 0.000
 LIMIT= 1000.000 K
 NO T-P DATA GRID
 0 SPECIES IN REACTION=
 0.000 XX 0.000 XX 0.000 XX
 LOG K= 500.000 DELHOR= 500.000 KCAL/MOL
 DELSOR= 500.000 CAL/MOL/K

* KIM (1983A), LOG K = 28.56 FOR AM+++ + 3OH- = AM(OH)3(C) AT I = 0.
 * SILVA (1982), LOG K = -16.6 FOR AM+++ + 3H2O = AM(OH)3(C) + 3H+
 * AT I = 0.1.
 * EDELSTEIN (1983), MEASURED SOLUBILITY OF SOLID THAT MAY HAVE BEEN
 * AM(OH)3; SOLID PHASE NOT IDENTIFIED.
 * USE DATA FROM KIM AND SILVA IN COMBINATION WITH ASSUMED HYDROLYSIS
 * PRODUCT CONSTANTS FROM MDAQSAM FILE TO MATCH SOLUBILITY.
 * LOG K = 27.8 FOR AM+++ + 3OH- = AM(OH)3(C) AT I = 0.

AM(OH)CO3(C)

ENTERED BY= J.F. KERRISK DATE= 09/01/83
 SOURCE= QUALITY=
 4 CHEMICAL ELEMENTS=
 1.000 AM 1.000 C 1.000 H
 4.000 O
 TEMP= 298.150 K PRESS= 1.000 BARS
 DELGO= -338.04 KCAL/MOL DELHO= 500.000 KCAL/MOL
 SO= 500.000 CAL/MOL/K VO= 0.000 CC/MOL
 1 HEAT CAPACITY RANGE(S) FOLLOW
 EQUATION= 0 CP OR A= 0.000 CAL/MOL/K
 B= 0.000 C= 0.000
 D= 0.000 E= 0.000
 LIMIT= 1000.000 K
 NO T-P DATA GRID
 0 SPECIES IN REACTION=
 0.000 XX 0.000 XX 0.000 XX
 LOG K= 500.000 DELHOR= 500.000 KCAL/MOL
 DELSOR= 500.000 CAL/MOL/K

* SILVA AND NITSCH (1983), LOG K = -2.67 FOR AM+++ + HCO3- + H2O =
 * AM(OH)CO3(C) + 2H+ AT I = 0.1.
 * KIM (1983B) HAS PROPOSED THIS SOLID ALSO, BUT NO DATA PUBLISHED.
 * USE DATA FROM SILVA AND NITSCH CORRECTED TO I = 0.

AM2(CO3)3(C)

ENTERED BY= J.F. KERRISK DATE= 09/01/83
 SOURCE= QUALITY=
 3 CHEMICAL ELEMENTS=
 2.000 AM 3.000 C 9.000 O
 TEMP= 298.150 K PRESS= 1.000 BARS
 DELGO= -716.100 KCAL/MOL DELHO= 500.000 KCAL/MOL
 SO= 500.000 CAL/MOL/K VO= 0.000 CC/MOL
 1 HEAT CAPACITY RANGE(S) FOLLOW
 EQUATION= 0 CP OR A= 0.000 CAL/MOL/K
 B= 0.000 C= 0.000
 D= 0.000 E= 0.000
 LIMIT= 1000.000 K
 NO T-P DATA GRID
 0 SPECIES IN REACTION=
 0.000 XX 0.000 XX 0.000 XX
 LOG K= 500.000 DELHOR= 500.000 KCAL/MOL
 DELSOR= 500.000 CAL/MOL/K

* SHILOH ET AL. (1969) MEASURED SOLUBILITY OF AMERICIUM IN HIGH
 * CARBONATE SOLUTIONS AND POSTULATED THIS SOLID PRECIPITATE.
 * DATA ESTIMATED FROM THEIR SOLUBILITY MEASUREMENTS.

* LOG K = 37.5 FOR 2AM+++ + 3CO3-- = AM2(CO3)3(C)
 * IDENTITY OF SOLID AND DATA ARE SPECULATIVE.

 AMO2(C)

ENTERED BY= J.F. KEFRISK DATE= 10/07/83
 SOURCE= QUALITY=
 2 CHEMICAL ELEMENTS= 2.000 O
 1.000 AM 2.000 O
 TEMP= 298.150 K PRESS= 1.000 BARS
 DELGO= 500.000 KCAL/MOL DELHO= 500.000 KCAL/MOL
 SO= 500.000 CAL/MOL/K VO= 0.000 CC/MOL
 1 HEAT CAPACITY RANGE(S) FOLLOW
 EQUATION= O CP OR A= 0.000 CAL/MOL/K
 B= 0.000 C= 0.000
 D= 0.000 E= 0.000
 LIMIT= 1000.000 K
 NO T-P DATA GRID
 0 SPECIES IN REACTION=
 0.000 XX 0.000 XX 0.000 XX
 LOG K= 500.000 DELHOR= 500.000 KCAL/MOL
 DELSOR= 500.000 CAL/MOL/K

*
 * KIM (1983A) DETERMINED SOLUBILITY UNDER UNKNOWN REDOX CONDITIONS;
 * CANNOT RELATE TO AM+++ CONCENTRATION.

 STOP.
 MDSOLAM

DATA ON MINERALS AND RELATED SUBSTANCES OF AMERICIUM

NOTATION--

-- DELGO = GIBBS ENERGY OF FORMATION
 -- DELGOR = GIBBS ENERGY OF REACTION
 -- DELHO = ENTHALPY OF FORMATION
 -- DELHOR = ENTHALPY OF REACTION
 -- SO = CONVENTIONAL ENTROPY
 -- DELSOR = ENTROPY OF REACTION

NOTE THAT "500." IS ENTERED TO MEAN "NO DATA" FOR DELGO, DELHO, SO, DELHTR, DELSTR, LOG K, DELHO, AND DELSOR. NEVER ENTER ZERO FOR THESE PARAMETERS OR LEAVE THEM BLANK UNLESS YOU MEAN TO USE AN ACTUAL VALUE OF ZERO. 1000 K IS THE DEFAULT FOR THE "LIMIT" PARAMETER.

IONIC STRENGTH CORRECTIONS WERE MADE USING THE DAVIES EQUATION IN THE FORM

$\text{LOG}(\text{GAMMA}) = 0.51 \cdot (Z^2) \cdot ((\text{SORT}(I)) / (1 + \text{SORT}(I))) - (0.2 \cdot I)$
 WHERE GAMMA IS THE ACTIVITY COEFFICIENT, Z IS THE CHARGE, AND I IS THE IONIC STRENGTH.

DATA FOR SOLID/GAS SPECIES=

NAME= AN ALPHABETIC OR ALPHANUMERIC STRING; E.G., CALCITE, BISCHOFITE.

THE FORMULA MAY ALSO BE USED AS THE NAME.

FORMULA= AN ALPHANUMERIC STRING DENOTING THE FORMULA OF THE SPECIES;

E.G., CaCO3, MgCl2.6H2O.

ENTERED BY= NAME OF PERSON WHO ENTERED DATA OR LAST REVISED IT

DATE= DATA OF ENTERING OR REVISING DATA

SOURCE= ALPHANUMERIC STRING IDENTIFYING A MAJOR SOURCE OF DATA. USE "SEE BELOW" FOR MINOR SOURCES

QUALITY= ALPHANUMERIC STRING DESCRIBING THE PROBABLE ERROR IN GIBBS ENERGY OR ITS EQUIVALENT, BASED ON SUBJECTIVE JUDGEMENT AND CHOSEN FROM AMONG THE FOLLOWING (IN ORDER OF INCREASING VALUE)

BAD - DEMONSTRABLY BAD DATA- DO NOT USE EXCEPT IN ILLUSTRATIVE CALCULATIONS

POOR - LIKELY ERROR EXCEEDS A COUPLE OF KCAL OR SEVERAL KJ

RESTRICTED - AD HOC FIT TO A PARTICULAR SITUATION; SEE NOTES

SPECULATIVE - SPECIES NOT SHOWN CONCLUSIVELY TO EXIST

UNCERTAIN - CHOSEN RATHER ARBITRARILY FROM DIVERGENT REPORTED VALUES

UNSPECIFIED - NO QUALITY INFORMATION

(BLANK) - EQUIVALENT TO UNSPECIFIED

FAIR - LIKELY ERROR LESS THAN A COUPLE OF KCAL OR A FEW KJ

GOOD - LIKELY ERROR LESS THAN ABOUT ONE KCAL OR FOUR KJ

THE CODE MUST BE MODIFIED TO ALLOW OTHER QUALITY PARAMETER INPUTS.

UNRECOGNIZED INPUTS ARE SET TO "ERROR". DATA FOR WHICH THE QUALITY IS "RESTRICTED", "SPECULATIVE", OR "UNCERTAIN" MAY NUMERICALLY BE "FAIR" TO "GOOD". THE MAJOR UNCERTAINTY ASSOCIATED WITH THESE VALUES IS QUALITATIVE (I.E., UNCERTAINTY OF INTERPRETATION). DATA FOR WHICH THE QUALITY IS "POOR" MAY BE QUITE SUFFICIENT FOR MAKING "GOOD" CALCULATIONS- THIS DEPENDS ON THE SENSITIVITY OF THE RESULTS TO IT IN ANY PARTICULAR APPLICATION.

NUMBER OF CHEMICAL ELEMENTS PER MOLE
 NUMBER OF MOLES OF ELEMENT PER MOLE OF SUBSTANCE
 SYMBOL OF CHEMICAL ELEMENT
 TEMP= THE BASE POINT TEMPERATURE (K), USUALLY 298.15 K
 PRESS= THE BASE POINT PRESSURE (BARS), USUALLY 1. BAR
 DELGO= THE APPARENT STANDARD PARTIAL MOLAL GIBBS ENERGY AT THE BASE POINT
 DELHO= THE APPARENT STANDARD PARTIAL MOLAL ENTHALPY AT THE BASE POINT
 SO= THE CONVENTIONAL ENTROPY AT THE BASE POINT
 VO= THE MOLAR VOLUME AT THE BASE POINT
 NUMBER OF HEAT CAPACITY RANGES THAT FOLLOW
 EQUATION= HEAT CAPACITY EQUATION CODE
 0- $CP = A + 1.E-3*B*T + 1.E+5*C*T**(-2) + 1.E-6*D*T**2$
 1- $CP = A + 1.E-3*B*T + 1.E+5*C*T**(-2) + 1.E+8*D*T**(-3)$
 CP= THE MOLAR HEAT CAPACITY, ASSUMED TO BE A CONSTANT
 A= FIRST HEAT CAPACITY COEFFICIENT
 B= SECOND HEAT CAPACITY COEFFICIENT
 C= THIRD HEAT CAPACITY COEFFICIENT
 D= FOURTH HEAT CAPACITY COEFFICIENT
 E= FIFTH HEAT CAPACITY COEFFICIENT
 LIMIT= UPPER LIMIT (K) OF THE PRECEDING SET OF HEAT CAPACITY PARAMETERS;
 NO T-P DATA GRID
 THIS IS EITHER THE UPPER LIMIT OF USE BASED ON THE RANGE OF MEASUREMENT OR THE TEMPERATURE OF A PHASE TRANSITION
 DELHTR= ENTHALPY OF A PHASE TRANSITION, IF ANY
 DELSTR= ENTROPY OF A PHASE TRANSITION, IF ANY
 T-P DATA GRID INDICATION LINE, FOLLOWED BY T-P DATA GRID, IF ANY
 TEMP, PRESS, DELGO, DELHO, SO, VO
 NUMBER OF SPECIES APPEARING IN A REACTION, IF A REACTION FOLLOWS
 NUMBER OF MOLES OF A SPECIES APPEARING IN THE REACTION
 THE NAME OF THE CORRESPONDING SPECIES
 LOG K= LOG OF THE EQUILIBRIUM CONSTANT OF THE GIVEN REACTION AT THE BASE POINT
 DELHOR= ENTHALPY OF THE GIVEN REACTION AT THE BASE POINT
 DELSOR= ENTROPY OF THE GIVEN REACTION AT THE BASE POINT

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- STOP.

APPENDIX C

Appendix C contains a listing of the input file REAC for the MCRT program. This file defines the chemical reactions of americium species that were considered.

```

RUN BY= J. F. KERRISK
DATE= 09/01/83
O O O O O O O O
AQUEOUS SPECIES OF AMERICIUM 8/03/83
AM+++ 1
1.00000 AM+++
AM++++ 5
-1.00000 AM++++ -0.50000 H2O
1.00000 H+ 1.00000 AM+++
0.25000 O2(G)
AM02+ 5
-1.00000 AM02+ -2.00000 H+
1.00000 H2O 1.00000 AM+++
0.50000 O2(G)
AM02++ 5
-4.00000 AM02++ -4.00000 H+
2.00000 H2O 4.00000 AM+++
3.00000 O2(G)
AMOH++ 3
-1.00000 AMOH++ 1.00000 AM+++
1.00000 OH-
AM(OH)2+ 3
-1.00000 AM(OH)2+ 1.00000 AM+++
2.00000 OH-
AM(OH)3 3
-1.00000 AM(OH)3 1.00000 AM+++
3.00000 OH-
AMCO3+ 3
-1.00000 AMCO3+ 1.00000 AM+++
1.00000 CO3--
AM(CO3)2- 3
-1.00000 AM(CO3)2- 1.00000 AM+++
2.00000 CO3--
AM(CO3)3--- 3
-1.00000 AM(CO3)3--- 1.00000 AM+++
3.00000 CO3--
AM(OH)CO3 4
-1.00000 AM(OH)CO3 1.00000 AM+++
1.00000 OH- 1.00000 CO3--
AM(OH)2CO3- 4
-1.00000 AM(OH)2CO3- 1.00000 AM+++
2.00000 OH- 1.00000 CO3--
AM(OH)(CO3)2-- 4
-1.00000 AM(OH)(CO3)2-- 1.00000 AM+++
1.00000 OH- 2.00000 CO3--
AMHCO3++ 3
-1.00000 AMHCO3++ 1.00000 AM+++
1.00000 HCO3-
AM(HCO3)2+ 3
-1.00000 AM(HCO3)2+ 1.00000 AM+++
2.00000 HCO3-
AMF++ 3
-1.00000 AMF++ 1.00000 AM+++
1.00000 F-
AMF2+ 3
-1.00000 AMF2+ 1.00000 AM+++
2.00000 F-
AMF3 3
-1.00000 AMF3 1.00000 AM+++
3.00000 F-
AMCL++ 3
-1.00000 AMCL++ 1.00000 AM+++
1.00000 CL-
AMCL2+ 3
-1.00000 AMCL2+ 1.00000 AM+++
2.00000 CL-
AMSO4+ 3
-1.00000 AMSO4+ 1.00000 AM+++
1.00000 SO4--
AM(SO4)2- 3
-1.00000 AM(SO4)2- 1.00000 AM+++
2.00000 SO4--
AMH2PO4++ 3
-1.00000 AMH2PO4++ 1.00000 AM+++
1.00000 H2PO4-
AM(H2PO4)2+ 3
-1.00000 AM(H2PO4)2+ 1.00000 AM+++
2.00000 H2PO4-
AM(H2PO4)3 3
-1.00000 AM(H2PO4)3 1.00000 AM+++

```

3.00000 H2PO4-		
AM(H2PO4)4-	3	
-1.00000 AM(H2PO4)4-		1.00000 AM+++
4.00000 H2PO4-		
AMNO3++	3	
-1.00000 AMNO3++		1.00000 AM+++
1.00000 NO3-		
AM(NO3)2+	3	
-1.00000 AM(NO3)2+		1.00000 AM+++
2.00000 NO3-		
AMO2HCO3	3	
-1.00000 AMO2HCO3		1.00000 AMO2+
1.00000 HCO3-		
SOLIDS OF AMERICIUM		8/03/83
AM(OH)3(C)	3	
-1.00000 AM(OH)3(C)		1.00000 AM+++
3.00000 OH-		
AM(OH)CO3(C)	4	
-1.00000 AM(OH)CO3(C)		1.00000 AM+++
1.00000 OH-		1.00000 CO3--
AM2(CO3)3(C)	3	
-1.00000 AM2(CO3)3(C)		2.00000 AM+++
3.00000 CO3--		

STOP.

APPENDIX D

Appendix D contains a listing of the output file DFILE from the MCRT program. This file contains the equilibrium-constant data for the reactions specified in Appendix C.

**** AQUEOUS ****

AM+++

ENTERED BY= J. F. KERRISK DATE= 09/01/83
 SOURCE= MCRT.3230U03 QUALITY= GOOD
 CHARGE= 3.0 TITR. FACTOR= 0.0 EQ/MOL
 ION SIZE= 8.0 A HYDR. NUMBER= 0.0
 1 CHEMICAL ELEMENTS=
 1.000 AM
 1 SPECIES IN REACTION=
 1.000 AM+++
 * LOG K GRID (0-25-60-100/150-200-250-300 C) =
 115.5310 104.9634 92.8252 81.7070
 70.7079 61.9886 54.8845 48.9704
 * DELVR GRID (0-25-60-100/150-200-250-300 C) =
 0.0000 0.0000 0.0000 0.0000
 0.0000 0.0000 0.0000 0.0000
 * MCRT FILE MDAQSO.3230U02 , REV. 09/01/83, CRISS-COBLE METHOD
 * (QUALITY OF AM+++ DATA = GOOD)

AM++++

ENTERED BY= J. F. KERRISK DATE= 09/01/83
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED
 CHARGE= 4.0 TITR. FACTOR= 0.0 EQ/MOL
 ION SIZE= 11.0 A HYDR. NUMBER= 0.0
 1 CHEMICAL ELEMENTS=
 1.000 AM
 5 SPECIES IN REACTION=
 -1.000 AM++++ -.500 H2O 1.000 H+
 1.000 AM+++ .250 O2(G)
 * LOG K GRID (0-25-60-100/150-200-250-300 C) =
 19.4620 18.8062 18.0343 17.3090
 16.5681 15.9597 15.4548 15.0276
 * DELVR GRID (0-25-60-100/150-200-250-300 C) =
 0.0000 0.0000 0.0000 0.0000
 0.0000 0.0000 0.0000 0.0000
 * MCRT FILE MDAQSAM DATA F, REV. 10/04/83, CRISS-COBLE METHOD
 * (QUALITY OF AM++++ DATA = UNSPECIFIED)

AM02+

ENTERED BY= J. F. KERRISK DATE= 09/01/83
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED
 CHARGE= 1.0 TITR. FACTOR= 0.0 EQ/MOL
 ION SIZE= 4.0 A HYDR. NUMBER= 0.0
 2 CHEMICAL ELEMENTS=
 1.000 AM 2.000 O
 5 SPECIES IN REACTION=
 -1.000 AM02+ -2.000 H+ 1.000 H2O
 1.000 AM+++ .500 O2(G)
 * LOG K GRID (0-25-60-100/150-200-250-300 C) =
 18.2750 16.7018 14.9026 13.2254
 11.5162 10.1138 8.9127 7.8565
 * DELVR GRID (0-25-60-100/150-200-250-300 C) =
 0.0000 0.0000 0.0000 0.0000
 0.0000 0.0000 0.0000 0.0000
 * MCRT FILE MDAQSAM DATA F, REV. 10/04/83, CRISS-COBLE METHOD
 * (QUALITY OF AM02+ DATA = UNSPECIFIED)

AM02++

ENTERED BY= J. F. KERRISK DATE= 09/01/83
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED
 CHARGE= 2.0 TITR. FACTOR= 0.0 EQ/MOL
 ION SIZE= 5.0 A HYDR. NUMBER= 0.0
 2 CHEMICAL ELEMENTS=
 1.000 AM 2.000 O
 5 SPECIES IN REACTION=
 -4.000 AM02++ -4.000 H+ 2.000 H2O
 4.000 AM+++ 3.000 O2(G)
 * LOG K GRID (0-25-60-100/150-200-250-300 C) =
 98.2481 91.3093 83.3951 76.1488
 68.9628 63.2418 58.5271 54.5462
 * DELVR GRID (0-25-60-100/150-200-250-300 C) =
 0.0000 0.0000 0.0000 0.0000
 0.0000 0.0000 0.0000 0.0000
 * MCRT FILE MDAQSAM DATA F, REV. 10/04/83, CRISS-COBLE METHOD
 * (QUALITY OF AM02++ DATA = UNSPECIFIED)

AM0H++

ENTERED BY= J. F. KERRISK DATE= 09/01/83
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED

```

      CHARGE= 2.0          TITR. FACTOR= 0.0 EQ/MOL
      ION SIZE= 5.0 A      HYDR. NUMBER= 0.0
      3 CHEMICAL ELEMENTS=
      1.000 AM          1.000 D          1.000 H
      3 SPECIES IN REACTION=
      -1.000 AMOH++      1.000 AM+++      1.000 OH-
*   LOG K GRID (0-25-60-100/150-200-250-300 C) =
      -7.5615 -7.5615 500.0000 500.0000
      500.0000 500.0000 500.0000 500.0000
*   DELVR GRID (0-25-60-100/150-200-250-300 C) =
      0.0000 0.0000 0.0000 0.0000
      0.0000 0.0000 0.0000 0.0000
* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
* (QUALITY OF AMOH++      DATA = UNSPECIFIED )
+-----+
AM(OH)2+
      ENTERED BY= J. F. KERRISK          DATE= 09/01/83
      SOURCE= MCRT.3230U03          QUALITY= UNSPECIFIED
      CHARGE= 1.0          TITR. FACTOR= 0.0 EQ/MOL
      ION SIZE= 4.0 A      HYDR. NUMBER= 0.0
      3 CHEMICAL ELEMENTS=
      1.000 AM          2.000 D          2.000 H
      3 SPECIES IN REACTION=
      -1.000 AM(OH)2+      1.000 AM+++      2.000 OH-
*   LOG K GRID (0-25-60-100/150-200-250-300 C) =
      -13.7009 -13.7009 500.0000 500.0000
      500.0000 500.0000 500.0000 500.0000
*   DELVR GRID (0-25-60-100/150-200-250-300 C) =
      0.0000 0.0000 0.0000 0.0000
      0.0000 0.0000 0.0000 0.0000
* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
* (QUALITY OF AM(OH)2+      DATA = UNSPECIFIED )
+-----+
AM(OH)3
      ENTERED BY= J. F. KERRISK          DATE= 09/01/83
      SOURCE= MCRT.3230U03          QUALITY= UNSPECIFIED
      CHARGE= 0.0          TITR. FACTOR= 0.0 EQ/MOL
      ION SIZE= 4.0 A      HYDR. NUMBER= 0.0
      3 CHEMICAL ELEMENTS=
      1.000 AM          3.000 D          3.000 H
      3 SPECIES IN REACTION=
      -1.000 AM(OH)3      1.000 AM+++      3.000 OH-
*   LOG K GRID (0-25-60-100/150-200-250-300 C) =
      -18.8802 -18.8802 500.0000 500.0000
      500.0000 500.0000 500.0000 500.0000
*   DELVR GRID (0-25-60-100/150-200-250-300 C) =
      0.0000 0.0000 0.0000 0.0000
      0.0000 0.0000 0.0000 0.0000
* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
* (QUALITY OF AM(OH)3      DATA = UNSPECIFIED )
+-----+
AMCO3+
      ENTERED BY= J. F. KERRISK          DATE= 09/01/83
      SOURCE= MCRT.3230U03          QUALITY= UNSPECIFIED
      CHARGE= 1.0          TITR. FACTOR= 0.0 EQ/MOL
      ION SIZE= 4.0 A      HYDR. NUMBER= 0.0
      3 CHEMICAL ELEMENTS=
      1.000 AM          3.000 D          1.000 C
      3 SPECIES IN REACTION=
      -1.000 AMCO3+      1.000 AM+++      1.000 CO3--
*   LOG K GRID (0-25-60-100/150-200-250-300 C) =
      -7.6524 -7.6524 500.0000 500.0000
      500.0000 500.0000 500.0000 500.0000
*   DELVR GRID (0-25-60-100/150-200-250-300 C) =
      0.0000 0.0000 0.0000 0.0000
      0.0000 0.0000 0.0000 0.0000
* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
* (QUALITY OF AMCO3+      DATA = UNSPECIFIED )
+-----+
AM(CO3)2-
      ENTERED BY= J. F. KERRISK          DATE= 09/01/83
      SOURCE= MCRT.3230U03          QUALITY= UNSPECIFIED
      CHARGE= -1.0          TITR. FACTOR= 0.0 EQ/MOL
      ION SIZE= 4.0 A      HYDR. NUMBER= 0.0
      3 CHEMICAL ELEMENTS=
      1.000 AM          6.000 D          2.000 C
      3 SPECIES IN REACTION=
      -1.000 AM(CO3)2-      1.000 AM+++      2.000 CO3--
*   LOG K GRID (0-25-60-100/150-200-250-300 C) =
      -12.1675 -12.1675 500.0000 500.0000

```

```

      500.0000  500.0000  500.0000  500.0000
*   DELVR GRID (0-25-60-100/150-200-250-300 C) =
      0.0000  0.0000  0.0000  0.0000
      0.0000  0.0000  0.0000  0.0000
*   MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
*   (QUALITY OF AM(CO3)2- DATA = UNSPECIFIED )
+-----+
AM(CO3)3---
  ENTERED BY= J. F. KERRISK          DATE= 09/01/83
    SOURCE= MCRT.3230U03          QUALITY= UNSPECIFIED
    CHARGE= -3.0                  TITR. FACTOR= 0.0 EQ/MOL
    ION SIZE= 4.0 A              HYDR. NUMBER= 0.0
    3 CHEMICAL ELEMENTS=
      1.000 AM          3.000 C          9.000 O
    3 SPECIES IN REACTION=
      -1.000 AM(CO3)3---  1.000 AM+++  3.000 CO3--
*   LOG K GRID (0-25-60-100/150-200-250-300 C) =
      500.0000  500.0000  500.0000  500.0000
      500.0000  500.0000  500.0000  500.0000
*   DELVR GRID (0-25-60-100/150-200-250-300 C) =
      0.0000  0.0000  0.0000  0.0000
      0.0000  0.0000  0.0000  0.0000
*   MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
*   (QUALITY OF AM(CO3)3--- DATA = UNSPECIFIED )
+-----+
AM(OH)CO3
  ENTERED BY= J. F. KERRISK          DATE= 09/01/83
    SOURCE= MCRT.3230U03          QUALITY= UNSPECIFIED
    CHARGE= 0.0                  TITR. FACTOR= 0.0 EQ/MOL
    ION SIZE= 4.0 A              HYDR. NUMBER= 0.0
    4 CHEMICAL ELEMENTS=
      1.000 AM          4.000 O          1.000 H
      1.000 C
    4 SPECIES IN REACTION=
      -1.000 AM(OH)CO3  1.000 AM+++  1.000 OH-
      1.000 CO3--
*   LOG K GRID (0-25-60-100/150-200-250-300 C) =
      500.0000  500.0000  500.0000  500.0000
      500.0000  500.0000  500.0000  500.0000
*   DELVR GRID (0-25-60-100/150-200-250-300 C) =
      0.0000  0.0000  0.0000  0.0000
      0.0000  0.0000  0.0000  0.0000
*   MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
*   (QUALITY OF AM(OH)CO3 DATA = UNSPECIFIED )
+-----+
AM(OH)2CO3-
  ENTERED BY= J. F. KERRISK          DATE= 09/01/83
    SOURCE= MCRT.3230U03          QUALITY= UNSPECIFIED
    CHARGE= -1.0                  TITR. FACTOR= 0.0 EQ/MOL
    ION SIZE= 4.0 A              HYDR. NUMBER= 0.0
    4 CHEMICAL ELEMENTS=
      1.000 AM          5.000 O          2.000 H
      1.000 C
    4 SPECIES IN REACTION=
      -1.000 AM(OH)2CO3-  1.000 AM+++  2.000 OH-
      1.000 CO3--
*   LOG K GRID (0-25-60-100/150-200-250-300 C) =
      500.0000  500.0000  500.0000  500.0000
      500.0000  500.0000  500.0000  500.0000
*   DELVR GRID (0-25-60-100/150-200-250-300 C) =
      0.0000  0.0000  0.0000  0.0000
      0.0000  0.0000  0.0000  0.0000
*   MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
*   (QUALITY OF AM(OH)2CO3- DATA = UNSPECIFIED )
+-----+
AM(OH)(CO3)2--
  ENTERED BY= J. F. KERRISK          DATE= 09/01/83
    SOURCE= MCRT.3230U03          QUALITY= UNSPECIFIED
    CHARGE= -2.0                  TITR. FACTOR= 0.0 EQ/MOL
    ION SIZE= 4.0 A              HYDR. NUMBER= 0.0
    4 CHEMICAL ELEMENTS=
      1.000 AM          1.000 H          7.000 O
      2.000 C
    4 SPECIES IN REACTION=
      -1.000 AM(OH)(CO3)2  1.000 AM+++  1.000 OH-
      2.000 CO3--
*   LOG K GRID (0-25-60-100/150-200-250-300 C) =
      500.0000  500.0000  500.0000  500.0000
      500.0000  500.0000  500.0000  500.0000
*   DELVR GRID (0-25-60-100/150-200-250-300 C) =

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      0.0000      0.0000      0.0000      0.0000
      0.0000      0.0000      0.0000      0.0000
* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
* (QUALITY OF AM(OH)(CO3)2-- DATA = UNSPECIFIED )
+-----+
AMHCO3++
  ENTERED BY= J. F. KERRISK          DATE= 09/01/83
    SOURCE= MCRT.3230UO3          QUALITY= UNSPECIFIED
    CHARGE= 2.0                  TITR. FACTOR= 0.0 EQ/MOL
    ION SIZE= 5.0 A              HYDR. NUMBER= 0.0
    4 CHEMICAL ELEMENTS=
      1.000 AM                  1.000 H                  1.000 C
      3.000 O
    3 SPECIES IN REACTION=
      -1.000 AMHCO3++          1.000 AM+++          1.000 HCO3-
*   LOG K GRID (0-25-60-100/150-200-250-300 C) =
      500.0000  500.0000  500.0000  500.0000
      500.0000  500.0000  500.0000  500.0000
*   DELVR GRID (0-25-60-100/150-200-250-300 C) =
      0.0000    0.0000    0.0000    0.0000
      0.0000    0.0000    0.0000    0.0000
* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
* (QUALITY OF AMHCO3++ DATA = UNSPECIFIED )
+-----+
AM(HCO3)2+
  ENTERED BY= J. F. KERRISK          DATE= 09/01/83
    SOURCE= MCRT.3230UO3          QUALITY= UNSPECIFIED
    CHARGE= 1.0                  TITR. FACTOR= 0.0 EQ/MOL
    ION SIZE= 4.0 A              HYDR. NUMBER= 0.0
    4 CHEMICAL ELEMENTS=
      1.000 AM                  2.000 H                  2.000 C
      6.000 O
    3 SPECIES IN REACTION=
      -1.000 AM(HCO3)2+      1.000 AM+++          2.000 HCO3-
*   LOG K GRID (0-25-60-100/150-200-250-300 C) =
      500.0000  500.0000  500.0000  500.0000
      500.0000  500.0000  500.0000  500.0000
*   DELVR GRID (0-25-60-100/150-200-250-300 C) =
      0.0000    0.0000    0.0000    0.0000
      0.0000    0.0000    0.0000    0.0000
* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
* (QUALITY OF AM(HCO3)2+ DATA = UNSPECIFIED )
+-----+
AMF++
  ENTERED BY= J. F. KERRISK          DATE= 09/01/83
    SOURCE= MCRT.3230UO3          QUALITY= UNSPECIFIED
    CHARGE= 2.0                  TITR. FACTOR= 0.0 EQ/MOL
    ION SIZE= 5.0 A              HYDR. NUMBER= 0.0
    2 CHEMICAL ELEMENTS=
      1.000 AM                  1.000 F
    3 SPECIES IN REACTION=
      -1.000 AMF++          1.000 AM+++          1.000 F-
*   LOG K GRID (0-25-60-100/150-200-250-300 C) =
      -4.2246  -4.3004  -4.4779  -4.7507
      -5.1725  -5.6792  -6.3105  -7.1899
*   DELVR GRID (0-25-60-100/150-200-250-300 C) =
      0.0000    0.0000    0.0000    0.0000
      0.0000    0.0000    0.0000    0.0000
* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, CRISS-COBBLE METHOD
* (QUALITY OF AMF++ DATA = UNSPECIFIED )
+-----+
AMF2+
  ENTERED BY= J. F. KERRISK          DATE= 09/01/83
    SOURCE= MCRT.3230UO3          QUALITY= UNSPECIFIED
    CHARGE= 1.0                  TITR. FACTOR= 0.0 EQ/MOL
    ION SIZE= 4.0 A              HYDR. NUMBER= 0.0
    2 CHEMICAL ELEMENTS=
      1.000 AM                  2.000 F
    3 SPECIES IN REACTION=
      -1.000 AMF2+          1.000 AM+++          2.000 F-
*   LOG K GRID (0-25-60-100/150-200-250-300 C) =
      -7.3987  -7.3987  500.0000  500.0000
      500.0000  500.0000  500.0000  500.0000
*   DELVR GRID (0-25-60-100/150-200-250-300 C) =
      0.0000    0.0000    0.0000    0.0000
      0.0000    0.0000    0.0000    0.0000
* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
* (QUALITY OF AMF2+ DATA = UNSPECIFIED )
+-----+
AMF3

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ENTERED BY= J. F. KERRISK          DATE= 09/01/83
SOURCE= MCRT.3230U03              QUALITY= UNSPECIFIED
CHARGE= 0.0                        TITR. FACTOR= 0.0 EQ/MOL
ION SIZE= 4.0 A                    HYDR. NUMBER= 0.0
2 CHEMICAL ELEMENTS=
1.000 AM                          3.000 F
3 SPECIES IN REACTION=
-1.000 AMF3                        1.000 AM+++      3.000 F-
* LOG K GRID (0-25-60-100/150-200-250-300 C) =
-10.5997 -10.5997 500.0000 500.0000
500.0000 500.0000 500.0000 500.0000
* DELVR GRID (0-25-60-100/150-200-250-300 C) =
0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000
* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
* (QUALITY OF AMF3 DATA = UNSPECIFIED )
+-----+
AMCL++
ENTERED BY= J. F. KERRISK          DATE= 09/01/83
SOURCE= MCRT.3230U03              QUALITY= UNSPECIFIED
CHARGE= 2.0                        TITR. FACTOR= 0.0 EQ/MOL
ION SIZE= 5.0 A                    HYDR. NUMBER= 0.0
2 CHEMICAL ELEMENTS=
1.000 AM                          1.000 CL
3 SPECIES IN REACTION=
-1.000 AMCL++                     1.000 AM+++      1.000 CL-
* LOG K GRID (0-25-60-100/150-200-250-300 C) =
-1.0995 -1.0995 500.0000 500.0000
500.0000 500.0000 500.0000 500.0000
* DELVR GRID (0-25-60-100/150-200-250-300 C) =
0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000
* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
* (QUALITY OF AMCL++ DATA = UNSPECIFIED )
+-----+
AMCL2+
ENTERED BY= J. F. KERRISK          DATE= 09/01/83
SOURCE= MCRT.3230U03              QUALITY= UNSPECIFIED
CHARGE= 1.0                        TITR. FACTOR= 0.0 EQ/MOL
ION SIZE= 4.0 A                    HYDR. NUMBER= 0.0
2 CHEMICAL ELEMENTS=
1.000 AM                          2.000 CL
3 SPECIES IN REACTION=
-1.000 AMCL2+                     1.000 AM+++      2.000 CL-
* LOG K GRID (0-25-60-100/150-200-250-300 C) =
-1.5613 -1.5613 500.0000 500.0000
500.0000 500.0000 500.0000 500.0000
* DELVR GRID (0-25-60-100/150-200-250-300 C) =
0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000
* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
* (QUALITY OF AMCL2+ DATA = UNSPECIFIED )
+-----+
AMSO4+
ENTERED BY= J. F. KERRISK          DATE= 09/01/83
SOURCE= MCRT.3230U03              QUALITY= UNSPECIFIED
CHARGE= 1.0                        TITR. FACTOR= 0.0 EQ/MOL
ION SIZE= 4.0 A                    HYDR. NUMBER= 0.0
3 CHEMICAL ELEMENTS=
1.000 AM                          4.000 D          1.000 S
3 SPECIES IN REACTION=
-1.000 AMSO4+                     1.000 AM+++      1.000 SO4--
* LOG K GRID (0-25-60-100/150-200-250-300 C) =
-3.5982 -3.5982 500.0000 500.0000
500.0000 500.0000 500.0000 500.0000
* DELVR GRID (0-25-60-100/150-200-250-300 C) =
0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000
* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
* (QUALITY OF AMSO4+ DATA = UNSPECIFIED )
+-----+
AM(SO4)2-
ENTERED BY= J. F. KERRISK          DATE= 09/01/83
SOURCE= MCRT.3230U03              QUALITY= UNSPECIFIED
CHARGE= -1.0                       TITR. FACTOR= 0.0 EQ/MOL
ION SIZE= 4.0 A                    HYDR. NUMBER= 0.0
3 CHEMICAL ELEMENTS=
1.000 AM                          8.000 O          2.000 S
3 SPECIES IN REACTION=
-1.000 AM(SO4)2-                  1.000 AM+++      2.000 SO4--

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*   LOG K GRID (0-25-60-100/150-200-250-300 C) =
      -4.9975   -4.9975   500.0000   500.0000
      500.0000   500.0000   500.0000   500.0000
*   DELVR GRID (0-25-60-100/150-200-250-300 C) =
      0.0000     0.0000     0.0000     0.0000
      0.0000     0.0000     0.0000     0.0000
*   MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
*   (QUALITY OF AM(SO4)2- DATA = UNSPECIFIED )
+-----+
AMH2PD4++
  ENTERED BY= J. F. KERRISK          DATE= 09/01/83
  SOURCE= MCRT.3230U03              QUALITY= UNSPECIFIED
  CHARGE= 2.0                      TITR. FACTOR= 0.0 EQ/MOL
  ION SIZE= 5.0 A                   HYDR. NUMBER= 0.0
  4 CHEMICAL ELEMENTS=
    1.000 AM                        4.000 D                        1.000 P
    2.000 H
  3 SPECIES IN REACTION=
    -1.000 AMH2PD4++              1.000 AM+++              1.000 H2PD4-
*   LOG K GRID (0-25-60-100/150-200-250-300 C) =
      -2.7267   -2.7267   500.0000   500.0000
      500.0000   500.0000   500.0000   500.0000
*   DELVR GRID (0-25-60-100/150-200-250-300 C) =
      0.0000     0.0000     0.0000     0.0000
      0.0000     0.0000     0.0000     0.0000
*   MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
*   (QUALITY OF AMH2PD4++ DATA = UNSPECIFIED )
+-----+
AM(H2PD4)2+
  ENTERED BY= J. F. KERRISK          DATE= 09/01/83
  SOURCE= MCRT.3230U03              QUALITY= UNSPECIFIED
  CHARGE= 1.0                      TITR. FACTOR= 0.0 EQ/MOL
  ION SIZE= 4.0 A                   HYDR. NUMBER= 0.0
  4 CHEMICAL ELEMENTS=
    1.000 AM                        8.000 D                        2.000 P
    4.000 H
  3 SPECIES IN REACTION=
    -1.000 AM(H2PD4)2+            1.000 AM+++              2.000 H2PD4-
*   LOG K GRID (0-25-60-100/150-200-250-300 C) =
      -3.7162   -3.7162   500.0000   500.0000
      500.0000   500.0000   500.0000   500.0000
*   DELVR GRID (0-25-60-100/150-200-250-300 C) =
      0.0000     0.0000     0.0000     0.0000
      0.0000     0.0000     0.0000     0.0000
*   MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
*   (QUALITY OF AM(H2PD4)2+ DATA = UNSPECIFIED )
+-----+
AM(H2PD4)3
  ENTERED BY= J. F. KERRISK          DATE= 09/01/83
  SOURCE= MCRT.3230U03              QUALITY= UNSPECIFIED
  CHARGE= 0.0                      TITR. FACTOR= 0.0 EQ/MOL
  ION SIZE= 4.0 A                   HYDR. NUMBER= 0.0
  4 CHEMICAL ELEMENTS=
    1.000 AM                        12.000 D                       3.000 P
    6.000 H
  3 SPECIES IN REACTION=
    -1.000 AM(H2PD4)3            1.000 AM+++              3.000 H2PD4-
*   LOG K GRID (0-25-60-100/150-200-250-300 C) =
      -4.6911   -4.6911   500.0000   500.0000
      500.0000   500.0000   500.0000   500.0000
*   DELVR GRID (0-25-60-100/150-200-250-300 C) =
      0.0000     0.0000     0.0000     0.0000
      0.0000     0.0000     0.0000     0.0000
*   MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
*   (QUALITY OF AM(H2PD4)3 DATA = UNSPECIFIED )
+-----+
AM(H2PD4)4-
  ENTERED BY= J. F. KERRISK          DATE= 09/01/83
  SOURCE= MCRT.3230U03              QUALITY= UNSPECIFIED
  CHARGE= -1.0                     TITR. FACTOR= 0.0 EQ/MOL
  ION SIZE= 4.0 A                   HYDR. NUMBER= 0.0
  4 CHEMICAL ELEMENTS=
    1.000 AM                        16.000 D                       4.000 P
    8.000 H
  3 SPECIES IN REACTION=
    -1.000 AM(H2PD4)4-            1.000 AM+++              4.000 H2PD4-
*   LOG K GRID (0-25-60-100/150-200-250-300 C) =
      -5.2408   -5.2408   500.0000   500.0000
      500.0000   500.0000   500.0000   500.0000
*   DELVR GRID (0-25-60-100/150-200-250-300 C) =

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0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000
* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
* (QUALITY OF AM(H2PO4)4- DATA = UNSPECIFIED )
+-----+
AMND3++
ENTERED BY= J. F. KERRISK DATE= 09/01/83
SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED
CHARGE= 2.0 TITR. FACTOR= 0.0 EQ/MOL
ION SIZE= 5.0 A HYDR. NUMBER= 0.0
3 CHEMICAL ELEMENTS=
1.000 AM 3.000 D 1.000 N
3 SPECIES IN REACTION=
-1.000 AMND3++ 1.000 AM+++ 1.000 ND3-
* LOG K GRID (0-25-60-100/150-200-250-300 C) =
-1.1515 -1.1515 500.0000 500.0000
500.0000 500.0000 500.0000 500.0000
* DELVR GRID (0-25-60-100/150-200-250-300 C) =
0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000
* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
* (QUALITY OF AMND3++ DATA = UNSPECIFIED )
+-----+
AM(ND3)2+
ENTERED BY= J. F. KERRISK DATE= 09/01/83
SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED
CHARGE= 1.0 TITR. FACTOR= 0.0 EQ/MOL
ION SIZE= 4.0 A HYDR. NUMBER= 0.0
3 CHEMICAL ELEMENTS=
1.000 AM 6.000 D 2.000 N
3 SPECIES IN REACTION=
-1.000 AM(ND3)2+ 1.000 AM+++ 2.000 ND3-
* LOG K GRID (0-25-60-100/150-200-250-300 C) =
-1.6580 -1.6580 500.0000 500.0000
500.0000 500.0000 500.0000 500.0000
* DELVR GRID (0-25-60-100/150-200-250-300 C) =
0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000
* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
* (QUALITY OF AM(ND3)2+ DATA = UNSPECIFIED )
+-----+
AM02HCO3
ENTERED BY= J. F. KERRISK DATE= 09/01/83
SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED
CHARGE= 0.0 TITR. FACTOR= 0.0 EQ/MOL
ION SIZE= 4.0 A HYDR. NUMBER= 0.0
4 CHEMICAL ELEMENTS=
1.000 AM 1.000 H 1.000 C
5.000 D
3 SPECIES IN REACTION=
-1.000 AM02HCO3 1.000 AMD2+ 1.000 HCO3-
* LOG K GRID (0-25-60-100/150-200-250-300 C) =
-2.3001 -2.3001 500.0000 500.0000
500.0000 500.0000 500.0000 500.0000
* DELVR GRID (0-25-60-100/150-200-250-300 C) =
0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000
* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
* (QUALITY OF AM02HCO3 DATA = UNSPECIFIED )
+-----+
**** SOLIDS ****
+-----+
AM(OH)3(C)
ENTERED BY= J. F. KERRISK DATE= 09/01/83
SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED
VOLUME= 0.000 CC/MOL
3 CHEMICAL ELEMENTS=
1.000 AM 3.000 D 3.000 H
3 SPECIES IN REACTION=
-1.000 AM(OH)3(C) 1.000 AM+++ 3.000 OH-
* LOG K GRID (0-25-60-100/150-200-250-300 C) =
-27.8006 -27.8006 500.0000 500.0000
500.0000 500.0000 500.0000 500.0000
* DELVR GRID (0-25-60-100/150-200-250-300 C) =
0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000
* MCRT FILE MDSOLAM DAT, REV. 10/03/83, INSUFFICIENT DATA
* (QUALITY OF AM(OH)3(C) DATA = UNSPECIFIED )
+-----+
AM(OH)CO3(C)

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ENTERED BY= J. F. KERRISK          DATE= 09/01/83
SOURCE= MCRT.3230U03              QUALITY= UNSPECIFIED
VOLUME= 0.000 CC/MOL
4 CHEMICAL ELEMENTS=
  1.000 AM          1.000 C          1.000 H
  4.000 O
4 SPECIES IN REACTION=
  -1.000 AM(OH)CO3(C)  1.000 AM+++    1.000 OH-
  1.000 CO3--
* LOG K GRID (0-25-60-100/150-200-250-300 C) =
  -22.7709 -22.7709 500.0000 500.0000
  500.0000 500.0000 500.0000 500.0000
* DELVR GRID (0-25-60-100/150-200-250-300 C) =
  0.0000 0.0000 0.0000 0.0000
  0.0000 0.0000 0.0000 0.0000
* MCRT FILE MDSOLAM DAT, REV. 10/03/83, INSUFFICIENT DATA
* (QUALITY OF AM(OH)CO3(C) DATA = UNSPECIFIED )
+-----+
AM2(CO3)3(C)
ENTERED BY= J. F. KERRISK          DATE= 09/01/83
SOURCE= MCRT.3230U03              QUALITY= UNSPECIFIED
VOLUME= 0.000 CC/MOL
3 CHEMICAL ELEMENTS=
  2.000 AM          3.000 C          9.000 O
3 SPECIES IN REACTION=
  -1.000 AM2(CO3)3(C)  2.000 AM+++    3.000 CO3--
* LOG K GRID (0-25-60-100/150-200-250-300 C) =
  -37.5215 -37.5215 500.0000 500.0000
  500.0000 500.0000 500.0000 500.0000
* DELVR GRID (0-25-60-100/150-200-250-300 C) =
  0.0000 0.0000 0.0000 0.0000
  0.0000 0.0000 0.0000 0.0000
* MCRT FILE MDSOLAM DAT, REV. 10/03/83, INSUFFICIENT DATA
* (QUALITY OF AM2(CO3)3(C) DATA = UNSPECIFIED )
+-----+

```